ThermoBuild: Online Method Made Available for Accessing NASA Glenn Thermodynamic Data

NASA ThermoBuild

ThermoBuild is an interactive tool which uses the NASA Glenn Thermodynamic Database to select species and to obtain:

- 1. Tables of thermodynamic properties for a user-supplied temperature schedule
- 2. Data subsets for use in CEA, SUBEQ, or any other program. To generate a data subset, click here.

Click on symbols for atoms contained in desired compounds VA 5A IVA 4A VIIA 7A BA BA Allow ions: 100 VIB 6B VII8 IIB 2B 1B 1B 5B 36 Kr ж æ m 54 ď 67 69 Ce Gd 140.1 140.9 144.2 (147)150.4 152.0 157.3 158.9 162.5 164.9 167.3 168.9 173.0 175.0 101 103 Th Cm Ct Md Actinide Series~ No Pu Am Bk Es Fm (247)(247)(242)(243)(253)

Process

NASA ThermoBuild.

Long description. This screen capture shows NASA ThermoBuild, an interactive tool that uses the NASA Glenn Thermodynamic Database to select species and obtain (1) tables of thermodynamic properties for a user-supplied temperature schedule and (2) data subsets for use with CEA, SUBEQ, or any other computer program. Users can generate a data subset by selecting symbols from an online periodic table for atoms contained in desired compounds.

The new Web site program "ThermoBuild" allows users to easily access and use the NASA Glenn Thermodynamic Database of over 2000 solid, liquid, and gaseous species. A convenient periodic table allows users to "build" the molecules of interest and designate the temperature range over which thermodynamic functions are to be displayed. ThermoBuild also allows users to build custom databases for use with NASA's Chemical Equilibrium with Applications (CEA) program or other programs that require the NASA format for thermodynamic properties.

The NASA Glenn Research Center has long been a leader in the compilation and dissemination of up-to-date thermodynamic data, primarily for use with the NASA CEA program, but increasingly for use with other computer programs. The NASA Glenn Thermodynamic Database, available at http://www.grc.nasa.gov/WWW/CEAWeb/,

contains accurate, frequently updated thermodynamic data for over 2000 solid, liquid, and gaseous species (ref. 1). The data are presented as nine coefficients to an empirical formula in temperature for heat capacity, enthalpy, and entropy.

ThermoBuild is available as a link to the CEA Web site. It guides the user through the steps necessary to produce tabulated thermodynamic functions for one or several species without complicated calculations or interpolations. The user selects the constituent atoms from ThermoBuild's periodic table and is prompted for a temperature schedule. Heat capacity, enthalpy, entropy, Gibbs energy, heat of formation, and logK values are tabulated for the user's selected species. Equations and data references are conveniently available at the Web site.

Another useful feature of ThermoBuild allows users to create custom databases by downloading a subset of the NASA data. These custom databases can be used for specialty CEA applications, or for any program that requires the NASA empirical formula for thermodynamic properties.

ThermoBuild was made fully operational during fiscal year 2003. It was produced as part of a continuing program at Glenn to provide high-quality, easily accessible thermodynamic information to the scientific community.

Access the NASA Glenn Thermodynamic Database at http://www.grc.nasa.gov/WWW/CEAWeb/

Reference

 McBride, Bonnie J.; Zehe, Michael J.; and Gordon, Sanford: NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species. NASA/TP--2002-211556, 2002. http://gltrs.grc.nasa.gov/cgibin/GLTRS/browse.pl?2002 /TP-2002-211556.html

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